

Strained graphene in the presence of external probes

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We revise the tight binding approach to strained or curved graphene in the presence of external probes such as Photoemission or Scanning Tunneling Microscopy experiments. We show that extra terms arise in the continuum limit of the tight binding Hamiltonian which can not be accounted for by changes in the hopping parameters due to lattice deformations. These material independent extra couplings are of the same order of magnitude as the standard ones and have a geometric origin. Moreover, we show that no β -independent pseudomagnetic fields exist in strained graphene. The physical relevance of the extra terms to actual experiments involving local probes is discussed.

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One of the most interesting aspects of graphene is the tight relation between its morphological and electronic properties. Although this issue has been explored at length in the theoretical literature [1, 2], and there is a fair amount of related experiments [3–9], recent results [10–12] have given an extra push to the subject that will be explored in this work.

In the continuum limit of the standard tight binding (TB) approach, lattice deformations couple to the electronic excitations in the form of fictitious gauge fields or scalar potentials [2, 13]. The parameter that links the TB approach with the continuum elasticity theory, β , is related to the electron–phonon coupling and appears in the definition of the strain–induced fictitious fields. β reflects the changes in the hopping parameter t of the TB model with the changes of the relative distances between atomic nearest neighbors due to the lattice deformations. The continuum TB model has been very successful and has given rise to strain engineering in graphene [14–18]. The experimental observation of “pseudo Landau levels” associated to specific strain patterns [7, 10] has been modeled with the TB pseudomagnetic fields and constitutes a very beautiful experimental confirmation of the theory.

In a recent work [19] inspired by a geometric approach to curved graphene [20–24], the continuum TB Hamiltonian was supplemented with additional β -dependent terms arising from a higher order derivative expansion, which can be interpreted as a position-dependent Fermi velocity and an extra vector field. The presence of β in the coefficients of the strain–dependent terms is a consequence of the basic assumption of the discrete nearest neighbor TB approach, where the only parameter in the model is the hopping integral t_{ij} among nearest neighbors.

The issue of the possible relevance of the actual atomic positions to the TB Hamiltonian was raised in a recent publication [25], with the conclusion that an extra β -independent gauge field was needed to complete the model.

In this work we will complete the analysis of the continuum limit of the TB Hamiltonian that models the coupling of lattice deformations to electronic excitations in graphene, with special emphasis on the observational consequences for current experiments. We will derive additional β -independent terms needed to supplement the TB Hamiltonian in order to make a quantitative comparison with the experimental data when the continuum approximation is a good description. In particular we will show that, although the additional terms modify the coefficients of the position-dependent Fermi velocity and extra vector field obtained in [19], no β -independent pseudomagnetic fields [25] exist in strained graphene.

In what follows we will assume for simplicity that there are no short range interactions or disorder connecting the two Fermi points, so that the low energy description around each point remains valid. As is well known in the TB-elasticity approach [2, 26], elastic deformations of the lattice give rise, in the continuum limit, to pseudovector potentials that mimic the coupling of real magnetic fields to the electronic current. The standard TB Hamiltonian in the continuum limit is

$$H_{TB} = -iv_0 \int d^2x \psi^\dagger \sigma_j (\partial_j + iA_j) \psi. \quad (1)$$

where $v_0 = 3ta/2$ is the Fermi velocity for the perfect lattice, with t the hopping parameter for nearest neighbors and a the lattice constant; $j=1,2$ (summation over

a repeated index is understood over the article), and σ_j are the Pauli matrices. The pseudogauge potential A_j is related to the strain tensor by

$$A_1 = \frac{\beta}{2a}(u_{xx} - u_{yy}), \quad A_2 = \frac{\beta}{2a}(-2u_{xy}), \quad (2)$$

where $\beta = |\partial \log t / \partial \log a|$. The strain tensor is defined as $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h)$, where u_i and h are in- and out-of-plane displacements respectively. Note that one usually assumes that crystal deformations are small and (1) is valid only up to $O(u_{ij}^2)$ corrections. We will follow this practice for the rest of the paper.

The prefix “pseudo” reflects the fact that, unlike real magnetic fields, pseudomagnetic fields of elastic origin are invariant under time reversal and couple with opposite signs to the two Fermi points of the graphene system. In both cases, observable effects are not associated to the vector potential itself, but to the field $\vec{B} = \vec{\nabla} \times \vec{A}$. These are the vector fields giving rise to oscillations in the density of states discussed in the experiments [10, 11] and in the various works on strain engineering.

As shown in [19], if one uses the TB approach to go one order higher in the derivative expansion, the Hamiltonian (1) becomes

$$H_{TB} = -i \int d^2x \psi^\dagger [v_{ij}(x) \sigma_i \partial_j + v_0 \sigma_i \Gamma_i + iv_0 \sigma_i A_i] \psi, \quad (3)$$

where the field A_i is the one given in (2), v_{ij} is the tensorial and space dependent Fermi velocity, $v_{ij} = v_0 \left[\eta_{ij} - \frac{\beta}{4}(2u_{ij} + \eta_{ij} u_{kk}) \right]$, and Γ_i is a new vector field given by

$$\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij} = -\frac{\beta}{4} \left(\partial_j u_{ij} + \frac{1}{2} \partial_i u_{jj} \right). \quad (4)$$

The key observation in this paper is that TB Hamiltonians describing strained graphene [2, 26], and (3) in particular, are commonly derived in a specific reference system, the “crystal frame”. The reason is that the Bloch waves $a_k = \sum_x e^{-i\vec{k} \cdot \vec{x}} a_x$ used to diagonalize the TB hamiltonian are written using the atomic *equilibrium* positions $\{x\}$, which are regularly spaced and independent of the crystal deformation. On the other hand, in the presence of strain the positions measured in the “lab frame” are the actual positions of the atoms y_i . The two sets of coordinates are related by $y_i = x_i + u_i(x)$, where u_i is the in-plane horizontal displacement vector. Note that the vertical displacements h are identical in both systems. In the classical theory of elasticity, crystal (lab) frame coordinates are usually referred to as Lagrangian (Eulerian) coordinates [27].

Thus, the TB hamiltonian (3) is actually the crystal frame hamiltonian $H_c(x)$. In order to describe the interaction of electrons with external probes or fields, we must use the lab frame hamiltonian $H_{Lab}(y)$, i.e., the TB

Hamiltonian has to be rewritten in lab frame coordinates. The TB hamiltonian is the sum of the Dirac hamiltonian H_0 plus the terms induced by the lattice deformations. As these are already $O(u_{ij})$, we have to compute change-of-frame corrections only for the u_{ij} -independent piece $(H_0)_c$ of the crystal hamiltonian. The computation is simplified by using the symmetric convention for the derivatives of the fermion fields

$$(H_0)_c = -iv_0 \int d^2x \psi_c^\dagger(x) \sigma_i \overleftrightarrow{\partial}_i \psi_c(x) \quad (5)$$

where $\psi^\dagger \overleftrightarrow{\partial}_i \psi \equiv 1/2(\psi^\dagger \partial_i \psi - (\partial_i \psi^\dagger) \psi)$ and the subscript in ψ_c indicates that this is the fermion field operator in the crystal frame. The derivatives transform according to

$$\frac{\partial}{\partial x_i} = \frac{\partial y_k}{\partial x_i} \frac{\partial}{\partial y_k} = (\delta_{ik} + \partial_i u_k) \partial_k = (\delta_{ik} + \tilde{u}_{ik} + \omega \varepsilon_{ik}) \partial_k, \quad (6)$$

where $\tilde{u}_{ik} = (\partial_i u_k + \partial_k u_i)/2$ is the linear piece of the strain tensor and $\omega \varepsilon_{ik} = (\partial_i u_k - \partial_k u_i)/2$. We also have to transform the integration measure

$$\begin{aligned} d^2x &= \left| \det \left(\frac{\partial x_k}{\partial y_i} \right) \right| d^2y = |\det(\delta_{ik} - \tilde{u}_{ik} - \omega \varepsilon_{ik})| d^2y \\ &\simeq (1 - \tilde{u}_{ii}) d^2y. \end{aligned} \quad (7)$$

On the other hand, $\psi_c^\dagger \psi_c$ is the particle density operator in the crystal frame. As the number of fermions in any region should be frame independent, we must impose $\psi_c^\dagger \psi_c d^2x = \psi^\dagger \psi d^2y$, where $\psi(y)$ is the lab frame field operator. This implies

$$\psi_c(x) = \left| \det \left(\frac{\partial x_k}{\partial y_i} \right) \right|^{-1/2} \psi(y), \quad (8)$$

which exactly cancels the Jacobian in (7). The net result is

$$\begin{aligned} &-iv_0 \int d^2x \psi_c^\dagger(x) \sigma_i \overleftrightarrow{\partial}_i \psi_c(x) \simeq \\ &-iv_0 \int d^2y \left[\psi^\dagger(y) \sigma_i \overleftrightarrow{\partial}_i \psi(y) + (\tilde{u}_{kl} + \omega \varepsilon_{kl}) (\psi^\dagger \sigma_k \overleftrightarrow{\partial}_l \psi) \right], \end{aligned} \quad (9)$$

where the derivatives in the last term act only on the fermion fields. Finally, the dependence on the antisymmetric piece $\omega \varepsilon_{ij}$ may be eliminated by a local rotation of the pseudospinors

$$\psi(y) \rightarrow e^{-\frac{i}{2} \omega \sigma_3} \psi(y) \simeq \psi(y) - \frac{i}{2} \omega \sigma_3 \psi(y). \quad (10)$$

Indeed, the identity $i\sigma_k \sigma_3 = \varepsilon_{kl} \sigma_l$ shows that this rotation cancels the term proportional to ω in (9). A contribution proportional to $\partial_k \omega$ vanishes as well due to the

anticommutation relation $\{\sigma_3, \sigma_k\} = 0$ for $k = 1, 2$. This yields

$$H_{Lab} = H_{TB} + H_{Geom} \quad (11)$$

where H_{TB} is given by (3) and

$$\begin{aligned} H_{Geom} &= -iv_0 \int d^2x \tilde{u}_{kl} (\psi^\dagger \sigma_k \overleftrightarrow{\partial}_l \psi) \\ &= -iv_0 \int d^2x \psi^\dagger \left[\tilde{u}_{kl} \sigma_k \partial_l + \frac{1}{2} (\partial_l \tilde{u}_{kl}) \sigma_k \right] \psi. \end{aligned} \quad (12)$$

In the last line we have used integration by parts to revert to the asymmetric derivative convention. Note that, to first order in the strain, β -dependent terms are the same in both frames. Eqs. (11) and (12) are the main results in this paper.

As $\beta \simeq 2$, the new β -independent terms in H_{Geom} are of the same order of magnitude as those in the standard TB hamiltonian (3). In particular, the space-dependent Fermi velocity derived in the TB formalism in [19] will become

$$v_{ij} = v_0 \left[\delta_{ij} - \frac{\beta}{4} (2u_{ij} + \delta_{ij} u_{kk}) + \tilde{u}_{ij} \right] \quad (13)$$

with the corresponding correction for the vector field

$$\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij} = -\frac{\beta}{4} \left(\partial_j u_{ij} + \frac{1}{2} \partial_i u_{jj} \right) + \frac{1}{2} \partial_j \tilde{u}_{ij}. \quad (14)$$

Note, however, that these are not the only possible “frame effects” or consequences of the change of coordinates. Eqs. (11) and (12) give the Hamiltonian of isolated strained graphene. In order to couple the system to external fields such as electromagnetic waves in the continuum limit, one has to use the lab frame coordinates. Thus the substitution $\partial_l \rightarrow \partial_l - ieA_l^{ext}$ has to be made in the lab frame hamiltonian (11). This gives an additional strain-dependent but β -independent correction to the hamiltonian describing the interaction with an electromagnetic wave in the Coulomb gauge

$$\delta H_{int} = -v_0 e \int d^2x \tilde{u}_{kl} A_l^{ext} (\psi^\dagger \sigma_k \psi). \quad (15)$$

The hamiltonian H_{Lab} can also be obtained by performing the TB calculation directly in the lab frame. This derivation is explicitly given in the Supplemental Material, where a seemingly new additional pseudogauge field is shown to have zero curl. As Γ_i is the only “new” vector field in strained or curved graphene, in what follows we will comment briefly on its physical significance and compare it with the well known pseudogauge field A_i in Eq. (2). First of all, note that, unlike A_i , Γ_i is not a functionally independent field. The reason is that the hamiltonian (3) is hermitian only for $\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij}$.

Thus, a position dependent Fermi velocity requires the existence of the new vector field Γ_i .

A look at (3) suggests that Γ_i is some sort of purely imaginary [28] counterpart to A_i . However, this is obviously wrong, as gauge potentials have to be real (hermitian). The true nature of Γ_i is made apparent if we use the identity $i\sigma_k \sigma_3 = \varepsilon_{kl} \sigma_l$ to rewrite the relevant term as $-iv_0 \sigma_i \Gamma_i = v_0 \sigma_i \tilde{\Gamma}_i$, with

$$\tilde{\Gamma}_1 = \Gamma_2 \sigma_3, \quad \tilde{\Gamma}_2 = -\Gamma_1 \sigma_3. \quad (16)$$

Note that $\tilde{\Gamma}_i$ is matrix-valued and hermitian. This shows that the vector field Γ_i plays the role a hermitian connection for the $SO(2)$ group of local pseudospin rotations (10) generated by σ_3 . As a consequence, a position dependent Fermi velocity will be accompanied by pseudospin rotation (“pseudospin precession”), i.e., by electronic transitions between the two sublattices. This fact is even more obvious in the covariant model in [19], where Γ_i appears as the spin connection associated to fermions propagating in a curved background. Thus Γ_i is not a gauge field and can not give rise to the characteristic Landau levels of real or pseudo-magnetic fields. The only pseudogauge field in strained graphene is the well known A_i given by (2).

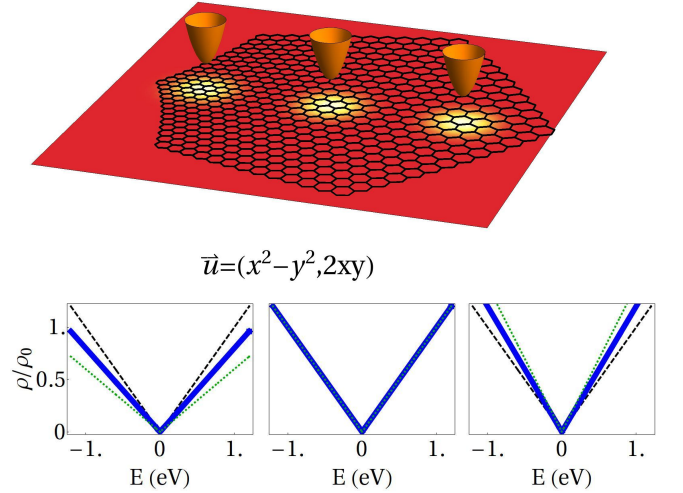


FIG. 1. Pictorial view of the strain field discussed in the text and the changes it produces in the density of states. The dotted (green) line represents the contribution from β dependent terms alone, while the thick (blue) line represents the total correction including frame effects. The three plots correspond to $x = -L, 0, L$ for the displacement discussed in the text with $u_{max} = 0.2$.

To see the practical implications of this work to actual measurements we now work out some practical examples. Consider first a density of states measurement. The frame effects discussed are rather trivial in this case

but enough to exemplify the issue. The effect of the coordinate change will affect STM measurements when the tip resolution is large in units of the lattice constant (no atomic resolution). The local density of states (LDOS) in the lab frame can be computed approximately in the local limit, for a sufficiently smooth u_{ij} . To do this, $\rho(E, u_{ij})$ is computed assuming u_{ij} is constant, and then its dependence on the position is restored in the final expression $\rho(E, x) \equiv \rho(E, u_{ij}(x))$. The LDOS can be computed in momentum space

$$\rho(E) = \int dq_x dq_y \text{tr}(E - H(q_x, q_y))^{-1} \quad (17)$$

with the Hamiltonian (11) by diagonalizing v_{ij} , which amounts to a change of integration variables

$$\rho(E) = \int \frac{dq_+ dq_-}{v_+ v_-} \text{tr}(E - H_0)^{-1}, \quad (18)$$

with H_0 the unperturbed Hamiltonian and v_{\pm} the velocity eigenvalues. This yields

$$\rho(E) = \frac{4}{2\pi} \frac{E}{v_+ v_-} = \rho_0(E) \frac{v_0^2}{v_+ v_-} \quad (19)$$

(the factor of 4 is due spin and valley degeneracy) which to first order in strain can be computed to give

$$\rho(E, x) = \rho_0(E) [(1 + \beta \text{tr } u - \text{tr } \tilde{u})]. \quad (20)$$

A simple but interesting example is provided by in-plane strains that are quadratic in the position, such as those associated to the triangular bumps that led to the observation of pseudo-Landau levels in STM [10] and that have been explicitly produced in artificial graphene in [11]. Remember that the TB gauge field associated to a strain tensor u_{ij} is $\vec{A} \propto (u_{xx} - u_{yy}, -2u_{xy})$. Consider first a deformation vector given by $\vec{u} = (x^2 - y^2, 2xy)u_{max}/4L$ shown in the upper part of Fig. 1. It is easy to see that the associated pseudomagnetic field will be zero in this case. The trace of the strain tensor is $\text{tr } u = u_{max}x/L$, hence a line scan along the y direction will give a perfect constant V shape ($\rho(E, x) \sim |E|$), while along the x direction there will be a dilatation effect such that $\rho(E, x) \sim (1 + u_{max}(\beta - 1)x/L)|E|$, as depicted in the lower part of Fig. 1 for different values of x . Due to the frame effects discussed in this work there is an additional, material independent change in the magnitude of the LDOS that adds on top of the β dependent contributions. This is important to consider if one wants to measure the space-dependent Fermi velocity from a local probe with resolution larger than the lattice constant.

An interesting thing happens if we now consider the same deformation vector but exchange u_x and u_y , i.e., $\vec{u} \propto (2xy, x^2 - y^2)$. In this case there will be no volume effect ($\text{tr } u = 0$) and the strain will give rise to a constant pseudomagnetic field whose associated density of

states will show similar Landau levels oscillations along any scanline. A 90 degree rotation of the strain deformation will give the same V shape with a Fermi velocity increasing this time along $x = \text{const}$. Finally, for the strain $\vec{u} \propto (x^2 - y^2, -2xy)$ both the trace and the pseudomagnetic field will be zero and there will be no effect altogether. It can be shown that the geometric vector field coming from the frame change does not affect the DOS at the linear order in u_{ij} considered in this work.

On the other hand, these examples are a simple illustration of the fact that the Honeycomb lattice is very anisotropic and, of course, does not have full rotational symmetry; hence similar looking deformations give rise to very different effects in the STM images. The important point is that, in the case of general strain, the frame effects discussed in this work will be responsible for additional spatial modulation of the intensity of the LDOS while preserving its energy dependence.

Frame effects will also be important when the absolute orientation of the lattice changes locally. An example of this effect can be observed in the polarization dependence of ARPES signal [29]. The usual ARPES pictures of Dirac cones see only one half of the cones, due to the form of the matrix element of the lattice electron at the K point with the free electron that comes out. This effect sees the absolute orientation of the lattice: if the lattice is rotated with respect to the polarization of light, the part of the Dirac cone that is observed also rotates. As before, in order to describe the physics in the lab frame, vectors in the crystal frame have to be rotated to the lab frame. This is again a β -independent contribution. Note, however, that the suppression of part of the observed Dirac cones in ARPES is due to the interference between photoelectrons emitted from the two sublattices and, as such, goes beyond the continuum limit interaction in (15). Effects of local lattice rotations in ARPES have been reported recently in [30]. The frame effects associated to lattice rotations could also be observed in optical experiments like those described in [31].

As a summary, we have shown that the TB description of deformed graphene in the continuum limit must be supplemented with geometric terms originating in the change of coordinates needed to describe interactions with external probes. These are of course always present in the experiments. The correct Hamiltonian to use when trying to fit experiments is $H_{lab} = H_{TB} + H_{Geom}$. The new terms are material independent and different from the usual gauge fields arising from deformation induced changes in the hopping parameter. The extra terms associated with these frame effects are of the same form as those already present in the complete TB Hamiltonian (3), but come with β -independent coefficients. Moreover, the only “new” vector field in strained graphene is the connection Γ_i (also present in the geometric formalism [19]), which is compatible with the symmetry analysis in [32–35] and required by the her-

miticity of the hamiltonian whenever we have a position dependent Fermi velocity. As discussed above, it is not a gauge field and will not give rise to Landau levels in the density of states, although it may have other physical effects, such as pseudospin precession. No material independent gauge fields having physical consequences arise in strained graphene. The frame effects described in this work will be relevant to local experiments with resolution $\lambda \gg a$, for which a continuum limit is appropriate.

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SUPPLEMENTAL MATERIAL

The tight binding derivation in the lab frame.—

The extra terms to be added to the standard TB calculation due to frame effects can also be obtained by redoing the TB calculation directly in the lab frame. That is, we consider the TB Hamiltonian $H = -\sum_{\langle ij \rangle} t_{ij} a_i^\dagger b_j + \text{h.c.}$, but now we map the labels to positions in the lab frame

$$H = -t \sum_{\vec{y}, n} a_{\vec{y}}^\dagger b_{\vec{y}+\vec{\delta}_n} + \text{h.c.}, \quad (21)$$

where $\vec{y} = \vec{x} + \vec{u}(x)$ with $\vec{x} = m_1 \vec{a}_1 + m_2 \vec{a}_2$, and $\vec{\delta}_n$ are the three nearest neighbour vectors (we follow ref. [19] for their definition and other conventions). As our interest here is in the β -independent terms generated by the change of frames, we have assumed that the hopping parameters t_{ij} take their equilibrium value t . The real meaning of the relabeling in (21) is that non-equilibrium atomic positions are used in the Fourier expansions

$$\begin{aligned} a_y^\dagger &= \sum_k e^{-i\vec{k} \cdot [\vec{x} + \vec{u}(x)]} a_k^\dagger, \\ b_{y+\delta_n} &= \sum_k e^{i\vec{k} \cdot [\vec{x} + \vec{\delta}_n + \vec{u}(x+\delta_n)]} b_k. \end{aligned} \quad (22)$$

Note that, due to the fact that crystal momentum \vec{k} is purely two-dimensional, only the in-plane components \vec{u} of a three-dimensional displacement $(\vec{u}(x), h(x))$ will appear in the Fourier expansions in (22). As a consequence, only the linear piece \tilde{u}_{ij} of the strain tensor can give rise to frame effects, while the out of plane contribution $\partial_i h \partial_j h$ does not play any role in this regard. The same conclusion was reached in the main text by noting that only \vec{u} enters the coordinate transformation that relates crystal and lab frames.

To see how this will change the effective theory at the K-point, it is instructive to analyze a_y further before computing the Hamiltonian. If we restrict the states to $\vec{k} = \vec{K} + \delta\vec{k}$ with $\delta k < \Lambda$, we get

$$a_y = e^{i\vec{K} \cdot \vec{x}} e^{i\vec{K} \cdot \vec{u}(x)} \sum_{\delta k}^{\Lambda} e^{i\delta\vec{k} \cdot \vec{x}} e^{i\delta\vec{k} \cdot \vec{u}(x)} a_k \quad (23)$$

and, comparing with the corresponding expression $a_x = e^{i(\vec{K} + \delta\vec{k}) \cdot \vec{x}} a_k$ in the crystal frame, we observe two new contributions. The first one is $e^{i\vec{K} \cdot \vec{u}(x)}$, which we can factor outside the integral. This is a trivial phase factor that can be reabsorbed into a_y by a local gauge transformation and has no effect on the physics. As shown below, if we do not reabsorb this phase, it will show up in the effective theory as a new gauge field $A_i = \partial_i(K_j u_j) = (\tilde{u}_{ij} + \omega \epsilon_{ij}) K_j$. But this gauge field has zero curl by construction and produces no pseudo-magnetic fields, even for position dependent strains. The second term $e^{i\delta\vec{k} \cdot \vec{u}(x_n)}$ cannot be eliminated by a gauge transformation in this way, and will induce extra terms in the Hamiltonian which precisely correspond to those in Eq. (9) after the field rescaling (8) is performed.

Back to the actual computation, plugging (22) into

(21) gives

$$H = -t \sum_{x,n} \sum_{k,k'} e^{-i\vec{k} \cdot (\vec{x} + \vec{u}(x))} e^{i\vec{k}' \cdot (\vec{x} + \vec{\delta}_n + \vec{u}(x+\delta_n))} a_k^\dagger b_{k'} + h.c. \quad (24)$$

It is convenient to use a symmetric parametrization for the momenta: $k \rightarrow k + q/2, k' \rightarrow k - q/2$, which corresponds to the symmetric derivative convention in (5). Expanding to linear order in u yields

$$\begin{aligned} H &= -t \sum_{x,n} \sum_{k,q} e^{-i\vec{q} \cdot \vec{x}} e^{i(\vec{k} - \vec{q}/2) \cdot \vec{\delta}_n} a_{k+q/2}^\dagger b_{k-q/2} \times \left[1 + \right. \\ &\quad \left. - \frac{i}{2} \vec{q} \cdot (\vec{u}(x) + \vec{u}(x + \delta_n)) - i\vec{k} \cdot (\vec{u}(x) - \vec{u}(x + \delta_n)) \right] + h.c. \end{aligned} \quad (25)$$

which, in terms of the Fourier coefficients of the displacement $u(x) = \sum_q e^{i\vec{q} \cdot \vec{x}} u(q)$ can be rewritten as

$$\begin{aligned} H &= -t \sum_{n,k,q} e^{i(\vec{k} - \vec{q}/2) \cdot \vec{\delta}_n} a_{k+q/2}^\dagger b_{k-q/2} \times \\ &\quad \left[\delta(\vec{q}) - \frac{i}{2} \vec{u}(q) \cdot \left(\vec{q}(1 + e^{i\vec{q} \cdot \vec{\delta}_n}) + 2\vec{k}(1 - e^{i\vec{q} \cdot \vec{\delta}_n}) \right) \right] + h.c. \end{aligned} \quad (26)$$

Expanding around the K-point and performing the sums over n as usual yields the matrix element

$$H_{k,q} = \frac{3ta}{2} [\delta(q) \sigma_i k_i + i q_i u_j(q) \sigma_i (K_j + k_j) - i q_i u_i(q) \sigma_j k_j], \quad (27)$$

where we have redefined $\delta k \rightarrow k$. Replacing $i q_i u_j(q) = \tilde{u}_{ij}(q) + \omega(q) \epsilon_{ij}$ we finally obtain

$$\begin{aligned} H_{k,q} &= v_0 [\delta(q) \sigma_i k_i + (\tilde{u}_{ij} + \omega \epsilon_{ij}) \sigma_i K_j \\ &\quad + (\tilde{u}_{ij} + \omega \epsilon_{ij}) \sigma_i k_j - \tilde{u}_{ii} \sigma_j k_j]. \end{aligned} \quad (28)$$

The last two terms are precisely those obtained from the direct coordinate transformation (6)-(7) of the continuum Dirac equation before the field rescaling (8), which eliminates the term proportional to \tilde{u}_{ii} . As anticipated, there is also a seemingly new gauge field

$$A_i = (\tilde{u}_{ij} + \omega \epsilon_{ij}) K_j = \partial_i (u_j K_j) \quad (29)$$

which is a total derivative and has zero associated magnetic field [36]. It can be eliminated by a local gauge transformation $\psi \rightarrow e^{-i\vec{K} \cdot \vec{u}(x)} \psi$.